

Hardcore dimer aspects of the SU(2) Singlet wavefunction

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We demonstrate that any SU(2) singlet wavefunction can be characterized by a set of Valence Bond occupation numbers, testing dimer presence/vacancy on pairs of sites. This genuine quantum property of singlet states (i) shows that SU(2) singlets share some of the intuitive features of hardcore quantum dimers, (ii) gives rigorous basis for interesting albeit apparently ill-defined quantities introduced recently in the context of Quantum Magnetism or Quantum Information to measure respectively spin correlations and bipartite entanglement and, (iii) suggests a scheme to define consistently a wide family of quantities analogous to high order spin correlation. This result is demonstrated in the framework of a general functional mapping between the Hilbert space generated by an arbitrary number of spins and a set of algebraic functions found to be an efficient analytical tool for the description of quantum spins or qubits systems.

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I. INTRODUCTION

Coupling a large number of spin $s = 1/2$ to a total spin $S = 0$ state (singlet) leads to a very rich class of wavefunctions which are the central pieces of many physical problems ranging from Condensed Matter to Quantum Information. Indeed, the singlet state plays a major role in Quantum Magnetism especially in the low temperature properties of SU(2) Heisenberg frustrated antiferromagnets : below the finite spin gap energy scale, the physics is dominated by rather exotic singlet ground states (valence bond crystal, plaquettes state, spin-liquid, ...) and often not so well understood low lying singlet excitations¹. It also attracted considerable interest since Anderson suggested that the Resonating Valence Bond (singlet) state (RVB) is the relevant insulating parent state of high- T_c superconductivity². Interestingly, these genuine quantum objects naturally emerge in the different context of Quantum Information because they are somehow paradigmatic of entanglement. Indeed, the simplest singlet ($S = 0$) wavefunction, namely the dimer state $(1/\sqrt{2})(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, is a maximally entangled state made out two spin $1/2$. For large systems, singlet wavefunction can naturally lead to massive entanglement³.

Obtaining a simple and tractable description of singlet states when the number of spins becomes large, is thus a crucial issue. In that respect, it has been shown since the early days of quantum mechanics that Valence Bond (VB) states⁴ are a much more convenient and elegant approach to this question than expansions of singlets as linear combinations of S_z eigenstates. Indeed, Hulthén showed⁵ that any singlet state can be written as a (non unique) linear combination of VB states, i.e. arbitrary range coverings of the N sites with dimers :

$$|\varphi_{\mathcal{D}}\rangle = \bigotimes_{(i,j) \in \mathcal{D}} [i, j], \quad (1)$$

where $[i, j] = (1/\sqrt{2})(|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle)$ and \mathcal{D} is a dimer covering of the system, defined as a partition of the $\{1, \dots, N\}$ ensemble into $N/2$ oriented couples of sites $\{(i_1, j_1), \dots, (i_{N/2}, j_{N/2})\}$ (see figure 1).

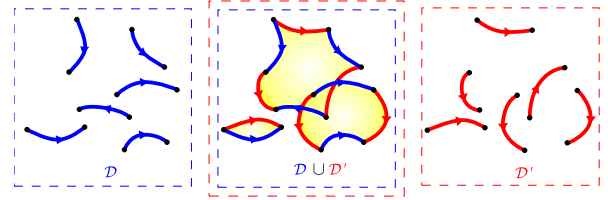


FIG. 1: Two VB states corresponding to the coverings \mathcal{D} and \mathcal{D}' . The overlap diagram obtained by the superimposition $\mathcal{D} \cup \mathcal{D}'$ involves a set a closed loops.

However, while emphasizing the role of an apparently intuitive source of spin correlation and entanglement (namely the “bond dimer” $(1/\sqrt{2})(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$), this approach leads to a non-orthogonal and massively overcomplete⁶ description of singlet states that, in turn, destroys any interpretation of dimers as hardcore objects⁷. Paradoxically enough, this conceptually problematic “dimer fuzziness” (caused by the intrinsic non-orthogonality of these objects) does not lead to major inconsistencies when neglected. Let us select three significant examples, from the contexts of Quantum Magnetism and Quantum Information, where this apparently ill-defined notion of bond occupation appears either implicitly or explicitly and is shown to give yet interesting and consistent results : (i) The Liang-Douçot-Anderson (LDA) wavefunction⁸ convincingly reinforces the idea that spin correlations can be driven by individual VB strength tuning, and in the same spirit Sandvik⁹ obtained very consistent results for the VB length distribution while mentioning the potential definition problem, (ii) The Rokhsar-Kivelson quantum dimer model¹⁰ that considers dimers as hardcore and orthogonal objects is widely accepted as a good starting point to the study of SU(2) highly frustrated (or more generally gapped) Heisenberg antiferromagnets^{11,12}, (iii) Alet *et al.*¹³ recently introduced a VB Entanglement Entropy numerically shown to capture all the features of the von Neumann Entanglement Entropy but defined as if dimers where hardcore and orthogonal objects.

In this article, we use a general functional framework to describe any singlet wavefunctions that allows to demonstrate that a VB occupation number testing the presence/absence of a

SU(2) dimer on a given pair of spins can be defined and computed unambiguously as an intrinsic property of any SU(2) singlet state. The implications are threefold: (i) We show that SU(2) singlets actually share some of the intuitive hardcore-like features of quantum dimers, (ii) We give rigorous basis for relevant albeit apparently ill-defined quantities introduced recently in the context of Quantum Magnetism such as VB Length Distribution⁹ or Quantum Information such as VB Entanglement Entropy¹³ and give a systematic scheme to define consistently a wide family of quantities analogous to high order spin correlation, (iii) The functional mapping provides a convenient framework for further studies of correlated and entangled quantum spin or qubits systems and can be extended to arbitrary values of spin s and total spin S .

The paper is organized as follow: in the first section we introduce and demonstrate the validity of the functional mapping. In the second part the VB occupation number is explicitly defined and shown to be the parent quantity for VB Length Distribution⁹ and VB Entanglement Entropy¹³. The final section is devoted to the generalization of the VB occupation number concept to arbitrary order VB correlation functions and the extension to higher spin s and total spin S values of the functional mapping.

II. FUNCTIONAL MAPPING

We introduce on each site i of the N -spin system a real (or complex) variable x_i and associate to any dimer covering \mathcal{D} the N -variable function $\varphi_{\mathcal{D}}$ defined by :

$$\varphi_{\mathcal{D}}(x_1, \dots, x_N) = \prod_{(i,j) \in \mathcal{D}} d(x_i, x_j), \quad (2)$$

where $d(x_i, x_j)$ is a function of x_i and x_j that will be determined later. Each function $\varphi_{\mathcal{D}}(\{x_i\})$ of the mapping corresponds to a pure VB state $|\varphi_{\mathcal{D}}\rangle$ defined by (1). The key properties of the VB states are their non-orthogonality and overcompleteness, both being closely related. Let us recall the overlap rule that allows to compute the overlap¹⁵ between two VB configurations \mathcal{D} and \mathcal{D}' ,

$$\mathcal{O}_{\mathcal{D}, \mathcal{D}'} = \langle \varphi_{\mathcal{D}} | \varphi_{\mathcal{D}'} \rangle = \varepsilon_{\mathcal{D}, \mathcal{D}'} 2^{n_l - N/2}, \quad (3)$$

n_l being the number of closed loops in the overlap diagram obtained by superimposing both configurations \mathcal{D} and \mathcal{D}' and $\varepsilon_{\mathcal{D}, \mathcal{D}'}$ the sign coming from the relative orientations of dimers in \mathcal{D} and \mathcal{D}' (see figure 1). The overcompleteness of the basis implies its non-orthogonality and on the other hand, all the linear relations between VB states are implicitly encoded into the overlap matrix \mathcal{O} : Because any singlet state can be expressed as a linear combination of arbitrary range VB states, the rank of \mathcal{O} is the singlet subspace size $\mathcal{N}_0 = N! / ((1 + N/2)!(N/2)!)$. Its size being $\mathcal{N} = N! / (2^{N/2}(N/2)!)$, all the overcompleteness of the basis is described by the $\mathcal{N} - \mathcal{N}_0$ independent singular eigenvectors of \mathcal{O} . Hence, in order to obtain a faithful functional representation, it is necessary and sufficient to determine $d(x_i, x_j)$ and define a scalar product $\langle \langle \varphi_{\mathcal{D}}(\{x_i\}) | \varphi_{\mathcal{D}'}(\{x_i\}) \rangle \rangle$ acting

on these functions that mimics the usual scalar product for VB states : $\langle \langle \varphi_{\mathcal{D}}(\{x_i\}) | \varphi_{\mathcal{D}'}(\{x_i\}) \rangle \rangle = \mathcal{O}_{\mathcal{D}, \mathcal{D}'}$.

Let us show that $d(x_i, x_j)$ can be chosen as

$$d(x_i, x_j) = \frac{1}{\sqrt{2}}(x_i - x_j), \quad (4)$$

and

$$\langle \langle \varphi_{\mathcal{D}}(\{x_i\}) | \varphi_{\mathcal{D}'}(\{x_i\}) \rangle \rangle = \sum_{x_i = \pm 1/2} \varphi_{\mathcal{D}}(\{x_i\}) \times \varphi_{\mathcal{D}'}(\{x_i\}). \quad (5)$$

Given the form (2), $\varphi_{\mathcal{D}}(\{x_i\}) \times \varphi_{\mathcal{D}'}(\{x_i\})$ involves bond terms and each variable x_i appears exactly twice. Hence, this term can be represented graphically by the set of even size closed loops of the overlap diagram (see figure 1). Loops being disconnected, $\langle \langle \varphi_{\mathcal{D}}(\{x_i\}) | \varphi_{\mathcal{D}'}(\{x_i\}) \rangle \rangle$ is just a product of the individual loop (l) traces contributions,

$$\langle \langle \varphi_{\mathcal{D}}(\{x_i\}) | \varphi_{\mathcal{D}'}(\{x_i\}) \rangle \rangle = \prod_{l \in \mathcal{D} \cup \mathcal{D}'} t_l \quad (6)$$

with, for a loop of size p ,

$$t_l = \sum_{x_i = \pm 1/2} d(x_{i_1}, x_{i_2}) d(x_{i_2}, x_{i_3}) \dots d(x_{i_p}, x_{i_1}). \quad (7)$$

Choosing (4) implies that only two sequences, $\{x_i\} = \{\pm 1/2, \mp 1/2, \dots, \mp 1/2\}$, give a non vanishing contribution to t_l . As a consequence, $t_l = 2 \cdot 2^{-p(l)/2} \cdot \varepsilon_l$ with $p(l)$ the size (number of sites) of the loop and $\varepsilon_l = \pm 1$ the contribution of the loop l to the global sign $\varepsilon_{\mathcal{D}, \mathcal{D}'} = \prod_{l \in \mathcal{D} \cup \mathcal{D}'} \varepsilon_l$. Because the total size of the loops is just the number of sites N , the overlap $\langle \langle \varphi_{\mathcal{D}}(\{x_i\}) | \varphi_{\mathcal{D}'}(\{x_i\}) \rangle \rangle = \varepsilon_{\mathcal{D}, \mathcal{D}'} 2^{n_l - N/2}$ as expected.

Using (5), we showed that the set of functions

$$\varphi_{\mathcal{D}}(x_1, \dots, x_N) = \frac{1}{2^{N/4}} \prod_{(i,j) \in \mathcal{D}} (x_i - x_j), \quad (8)$$

have the same linear properties as the VB states (1) and thus provides an algebraic mapping of the singlet subspace¹⁶.

We emphasize that this mapping is general as it establishes a one to one correspondence between any VB state (1) and its functional counterpart (8) : any subclass of VB states maps to its corresponding subclass both defining isomorphic Hilbert spaces. In the next section, we show (i) the particular role of the subset made of bipartite VB states, (ii) that valence bond occupation number is unambiguously defined using bipartite VB states despite non-orthogonality and overcompleteness.

III. VALENCE BOND OCCUPATION NUMBERS

Bipartition. The overcompleteness of the full VB basis prevents to define consistently a VB occupation number. We now show that such a definition is possible by restraining expansions of singlet states to a subset of \mathcal{V} , yet overcomplete and spanning all the singlet sector. Let us partition the N -spin system into two $N/2$ -spin subsets denoted \mathcal{A} and \mathcal{B} ¹⁷. We

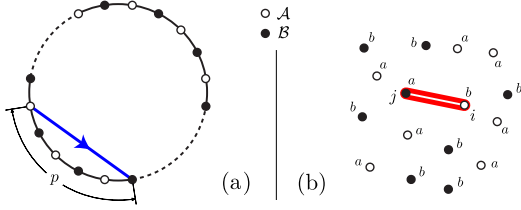


FIG. 2: (a) Arrangement of N spins around a circle, alternating \mathcal{A} sites and \mathcal{B} sites. (b) In the definition (14) of bond (i, j) occupation operator, the limit for x_k is taken to $a = 1/2$ for \mathcal{A} sites and $b \neq a$ for \mathcal{B} sites except for x_i and x_j for which the inverse convention is used: a if i (or j) is part of \mathcal{B} and b if i (or j) is part of \mathcal{A} .

consider the subset \mathcal{V}^b of \mathcal{V} containing the $\mathcal{N}^b = (N/2)!$ bipartite VB states :

$$|\varphi_{\mathcal{D}}\rangle = \bigotimes_{\substack{(i,j) \in \mathcal{D} \\ i \in \mathcal{A}, j \in \mathcal{B}}} [i, j]. \quad (9)$$

\mathcal{V}^b also provides an overcomplete description of the singlet subspace : let us arrange the N spins on a circle in such a way that \mathcal{A} sites alternate with \mathcal{B} sites (see figure 2 (a)) and choose an arbitrary singlet state $|\psi\rangle$. As shown by Rumer *et al.*⁴, there exist at least one decomposition of $|\psi\rangle$ as a linear combination of *non-crossing*¹⁸ VB states. A simple inspection at figure 2 (a) shows that these non-crossing states are also bipartite. The occurrence of a non-bipartite dimer would lead to the existence of an odd sized arc, hence causing at least one crossing. As a consequence any singlet state $|\psi\rangle$ can be written as,

$$|\psi\rangle = \sum_{\mathcal{D} \in \mathcal{V}^b} \lambda_{\mathcal{D}} |\varphi_{\mathcal{D}}\rangle. \quad (10)$$

This decomposition is not unique due to $\mathcal{N}^b - \mathcal{N}$ independent linear relations that reflect the overcompleteness of \mathcal{V}^b .

Bond Occupation. We denote by $n_{(i,j)}$ the occupation number of a bond (i, j) (bipartite or not) in a bipartite VB state $|\varphi_{\mathcal{D}}\rangle$ (9) and define it as,

$$n_{(i,j)}(|\varphi_{\mathcal{D}}\rangle) = \begin{cases} 1 & \text{if } (i, j) \text{ belongs to } \mathcal{D}, \\ 0 & \text{otherwise.} \end{cases} \quad (11)$$

For any singlet state $|\psi\rangle$ decomposed on \mathcal{V}^b as (10), we show that the bond occupation

$$n_{(i,j)}(|\psi\rangle) = \sum_{\mathcal{D} \in \mathcal{V}^b} \lambda_{\mathcal{D}} n_{(i,j)}(|\varphi_{\mathcal{D}}\rangle), \quad (12)$$

is *independent* of the decomposition (10) used, hence providing a consistent intrinsic definition of a bond occupation number for any singlet state. This statement is valid if any relation of overcompleteness implies its bond occupation counterpart :

$$\sum_{\mathcal{D} \in \mathcal{V}^b} \lambda_{\mathcal{D}} |\varphi_{\mathcal{D}}\rangle = 0 \Rightarrow \sum_{\mathcal{D} \in \mathcal{V}^b} \lambda_{\mathcal{D}} n_{(i,j)}(|\varphi_{\mathcal{D}}\rangle) = 0. \quad (13)$$

To demonstrate this point, let us use the functional mapping presented in the previous section and introduce the operator

$\mathcal{D}_{(i,j)}$ acting on the functions of the mapping,

$$\mathcal{D}_{(i,j)} f(\{x_k\}) = 2^{N/4} \lim_{\substack{x_i \rightarrow \alpha, x_j \rightarrow \beta \\ x_k \in \mathcal{A} \rightarrow 1/2 \\ x_k \in \mathcal{B} \rightarrow -1/2}} (\partial_{x_i} - \partial_{x_j}) f(\{x_k\}), \quad (14)$$

with α or $\beta = -1/2$ (resp. $+1/2$) if i or $j \in \mathcal{A}$ (resp. \mathcal{B}) (see figure 2 (b)). One can easily check that $\mathcal{D}_{(i,j)}$ have the following properties : (i) Linearity : $\mathcal{D}_{(i,j)}(f+g) = \mathcal{D}_{(i,j)}f + \mathcal{D}_{(i,j)}g$, (ii) For any $\mathcal{D} \in \mathcal{V}^b$, $\mathcal{D}_{(i,j)}\varphi_{\mathcal{D}} = 1$ if $(i, j) \in \mathcal{D}$ and $\mathcal{D}_{(i,j)}\varphi_{\mathcal{D}} = 0$ if $(i, j) \notin \mathcal{D}$. Using (8), l.h.s. of equation (13) becomes,

$$\sum_{\mathcal{D} \in \mathcal{V}^b} \lambda_{\mathcal{D}} \prod_{\substack{(p,q) \in \mathcal{D} \\ p \in \mathcal{A}, q \in \mathcal{B}}} (x_p - x_q) = 0, \quad (15)$$

and applying $\mathcal{D}_{(i,j)}$ to (15) immediately leads to the r.h.s. of (13) which concludes the demonstration.

At this point, it is important to mention that $n_{(i,j)}$ is reminiscent of a bond correlation $C_{ij} = (-4/3)\mathbf{S}_i \cdot \mathbf{S}_j$ but is *essentially different*. Indeed, $n_{(i,j)}^2(|\psi_{\mathcal{D}}\rangle) = \langle \varphi_{\mathcal{D}} | C_{ij} | \varphi_{\mathcal{D}} \rangle$ for any pure VB state. But, in the generic case of a superposition (10), both notions decouple due to the off-diagonal terms induced by the non-orthogonality of VB states :

$$\langle \psi | C_{ij} | \psi \rangle = n_{(i,j)}^2(|\psi\rangle) + \sum_{\substack{\mathcal{D}, \mathcal{D}' \\ \mathcal{D} \neq \mathcal{D}'}} \lambda_{\mathcal{D}} \lambda_{\mathcal{D}'} \langle \varphi_{\mathcal{D}'} | C_{ij} | \varphi_{\mathcal{D}} \rangle. \quad (16)$$

Illustration. For $N = 6$ (then $\mathcal{N}_0 = 5$, $\mathcal{N} = 15$ and $\mathcal{N}^b = 6$) we define the bipartite VB states taking $\mathcal{A} = \{1, 3, 5\}$ and $\mathcal{B} = \{2, 4, 6\}$. The overcomplete bipartite VB basis is : $|\alpha\rangle = [1, 2][3, 4][5, 6]$, $|\beta\rangle = [1, 6][3, 2][5, 4]$, $|\gamma\rangle = [1, 4][5, 2][3, 6]$, $|\delta\rangle = [1, 2][3, 6][5, 4]$, $|\varepsilon\rangle = [1, 4][3, 2][5, 6]$ and $|\zeta\rangle = [1, 6][5, 2][3, 4]$. The sole relation of overcompleteness writes $|\alpha\rangle + |\beta\rangle + |\gamma\rangle - |\delta\rangle - |\varepsilon\rangle - |\zeta\rangle = 0$. We can check that e.g. the occupation of bond $(5, 2)$ on the singlet state $3|\alpha\rangle + 2|\zeta\rangle$ that can be directly evaluated to $3 \times 0 + 2 \times 1 = 2$ is indeed independent of the decomposition : $3|\alpha\rangle + 2|\zeta\rangle = 5|\alpha\rangle + 2|\beta\rangle + 2|\gamma\rangle - 2|\delta\rangle - 2|\varepsilon\rangle$ leads to $5 \times 0 + 2 \times 0 + 2 \times 1 - 2 \times 0 - 2 \times 0 = 2$. On the other hand, the expectation value of $(-4/3)\mathbf{S}_2 \cdot \mathbf{S}_5$ is 5 and not $4 = 2^2$ for this state.

VB Length Distribution & VB Entanglement Entropy. Using this result any quantity built out from bond occupation/vacancy scheme on a singlet state $|\psi\rangle$ can be defined unambiguously. The VB Length Distribution computed in⁹ writes,

$$\mathcal{P}_l(|\psi\rangle) = \frac{\mathcal{L}_l(|\psi\rangle)}{\sum_l \mathcal{L}_l(|\psi\rangle)} \quad \text{with} \quad \mathcal{L}_l(|\psi\rangle) = \sum_{\substack{(i,j) \text{ with} \\ \text{length } l}} \mathcal{D}_{(i,j)}(|\psi\rangle), \quad (17)$$

where $\mathcal{L}_l(|\psi\rangle)$ is the total occupation of bonds with length l . A definition of the VB Entanglement Entropy introduced in¹³ as an equivalent of von Neumann Entanglement Entropy measurement of the bipartite entanglement between subsystems Ω and $\bar{\Omega}$ spanning the all system is,

$$S_{\Omega, \bar{\Omega}}^{\text{VB}}(|\psi\rangle) = \ln 2 \times \sum_{\substack{(i,j) \text{ crossing} \\ \Omega | \bar{\Omega}}} \mathcal{D}_{(i,j)}(|\psi\rangle). \quad (18)$$

IV. EXTENSIONS AND GENERALIZATIONS

VB correlation functions. Comparing (4) and (14) exhibit a duality in the mapping between the dimer representation ($x_i - x_j$) and a dimer susceptibility ($\partial_{x_i} - \partial_{x_j}$). It is then straightforward to introduce p -order VB occupation numbers (or *VB correlation functions*), similar to $2p$ -spin correlation functions, by defining *linear* operators in the spirit of (14) containing more than one bond susceptibility ($\partial_{x_{i_1}} - \partial_{x_{j_1}} \dots \partial_{x_{i_p}} - \partial_{x_{j_p}}$). The analogous of equation (16) for such an operator, shows that both quantities are equivalent for a pure VB state but becomes distinct yet consistently defined for a VB superposition. While much simpler to compute, we infer that VB correlation functions provide the same insights than usual correlations functions when computed on a given singlet state.

Higher total spin sectors for $s = 1/2$. Following Hulthén's scheme⁵ higher total spin S sectors with fixed total S_z can be (overcompletely) represented by introducing in the coverings (1) an arbitrary range totally symmetrized state of $2S$ spins $\{i_1, \dots, i_{2S}\}_{S_z}$. The functional mapping can be extended to these case in the spirit of (4) using the generating function $\mathcal{G}^S(\mu, \{x_{i_p}\}) = \prod_{p=1}^{2S} (1 + \mu x_{i_p})$ and representing $\{i_1, \dots, i_{2S}\}_{S_z}$ with

$$d_{S_z}^S(x_{i_1}, \dots, x_{i_{2S}}) = \sqrt{\frac{2^{2S_z} (S - S_z)!}{(2S)! (S + S_z)!}} \left(\partial_\mu^{(S_z+S)} \mathcal{G}^S \right) \Big|_{\mu=0}. \quad (19)$$

In particular $d_0^1(x_1, x_2) = (1/\sqrt{2})(x_i + x_j)$ represents the $S_z = 0$ bond triplet. Mixed total spin state such as the Néel state can be represented as well in this framework : If we denote \mathcal{A} the $N/2$ -site sublattice with up spins, it is easy to check that the corresponding Néel state is represented by $\Pi_{\mathcal{A}} = \prod_{i \in \mathcal{A}} x_i$ since, using (5), $\langle \langle \varphi_{\mathcal{D}}(\{x_i\}) | \Pi_{\mathcal{A}} \rangle \rangle = (1/2)^{N/4}$ for any bipartite \mathcal{D} .

Singlet sector for higher spins s . As noticed by Tasaki¹⁹, VB concept can be extended to higher values of s : $[i, j]_s = \frac{1}{\sqrt{2s+1}} \sum_{s_z=-s}^{+s} (-1)^{s-s_z} | -s_z, +s_z \rangle$. The overlap $\mathcal{O}_{\mathcal{D}, \mathcal{D}'}$ (3) becomes $\langle \varphi_{\mathcal{D}} | \varphi_{\mathcal{D}'} \rangle = \varepsilon_{\mathcal{D}, \mathcal{D}'} \cdot (2s+1)^{n_l - N/2}$ with $\varepsilon_{\mathcal{D}, \mathcal{D}'} =$

1 for integer s . It can be readily checked that choosing $d_s(x_i, x_j) = \frac{1}{\sqrt{2s+1}} (-1)^{s-x_i} \delta_{x_i, -x_j}$ and enlarging the support of the sum defining the scalar product (5) to $\sum_{x_i=-s}^{x_i=+s}$ leads to $\langle \langle \varphi_{\mathcal{D}}(\{x_i\}) | \varphi_{\mathcal{D}'}(\{x_i\}) \rangle \rangle = \langle \varphi_{\mathcal{D}} | \varphi_{\mathcal{D}'} \rangle$ thus providing the extension of the mapping. The proof that s -spins VB states provide an overcomplete description of the singlet sector (if N is large enough to ensure that the number of coverings is larger than size of the singlet sector) is beyond the scope of this article²⁰.

V. CONCLUSIONS

Any SU(2) singlet state can be characterized by a set of bond occupation numbers : despite the fuzziness induced by the overcompleteness of the VB basis, singlet wavefunctions conserve intuitive hardcore dimer features such as the possibility of deciding whether a SU(2) dimer live on a bond or not. This genuine quantum property formalizes the suggestive idea behind the LDA wavefunction⁸ that VB bond strength can drive the correlations properties of the singlet wavefunction and gives insights to the question of the interplay between non-orthogonality, overcompleteness and hardcore properties. Moreover, this allows consistent definitions of quantities relevant for Quantum Magnetism (VB Length Distribution⁹ and VB correlations¹⁴ of any order) or Quantum Information (VB Entanglement Entropy¹³) emphasizing the intuitive role of dimers as elementary bricks to build correlations or entanglement. We note that all these quantities are particularly suitable for numerical calculation in the framework introduced by Sandvik⁹. From a methodological point of view, the functional mapping used to derive this result appears as a suggestive tool to describe quantum spin or qubits systems and can be extended naturally to higher spins s and higher total spin S sectors.

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⁶ Indeed, the number of states in \mathcal{V} is $\mathcal{N} = N!/(2^{N/2}(N/2)!) \sim (N/e)^{N/2}$ which is much larger than the singlet subspace size $\mathcal{N}_0 = N!/((1+N/2)!(N/2)!) \sim 2^N/\sqrt{N}$.

⁷ Bond (1, 2) is occupied in the 4-spin singlet state $[1, 2][3, 4]$. But $[1, 2][3, 4] = [1, 3][2, 4] + [1, 4][3, 2]$, and the state can be expressed as a linear combination of VB states, none of them having bond (1, 2) occupied.

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- ¹⁶ As an illustration, one can easily check that the simplest over-completeness relation $[1, 2][3, 4] + [1, 3][4, 2] + [1, 4][2, 3] = 0$ is mapped the algebraic identity $(x_1 - x_2)(x_3 - x_4) + (x_1 - x_3)(x_4 - x_2) + (x_1 - x_4)(x_2 - x_3) = 0$.
- ¹⁷ Such a choice is always possible, since we do not presume any underlying geometry, lattice structure nor hamiltonian for the system.
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